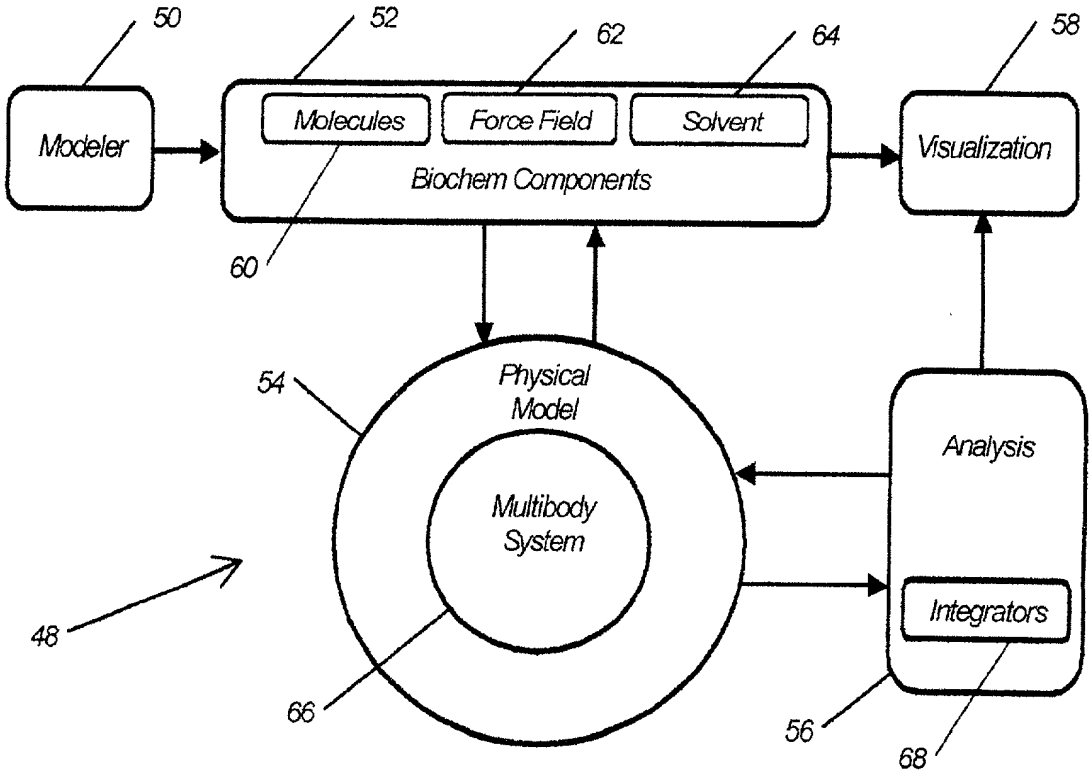
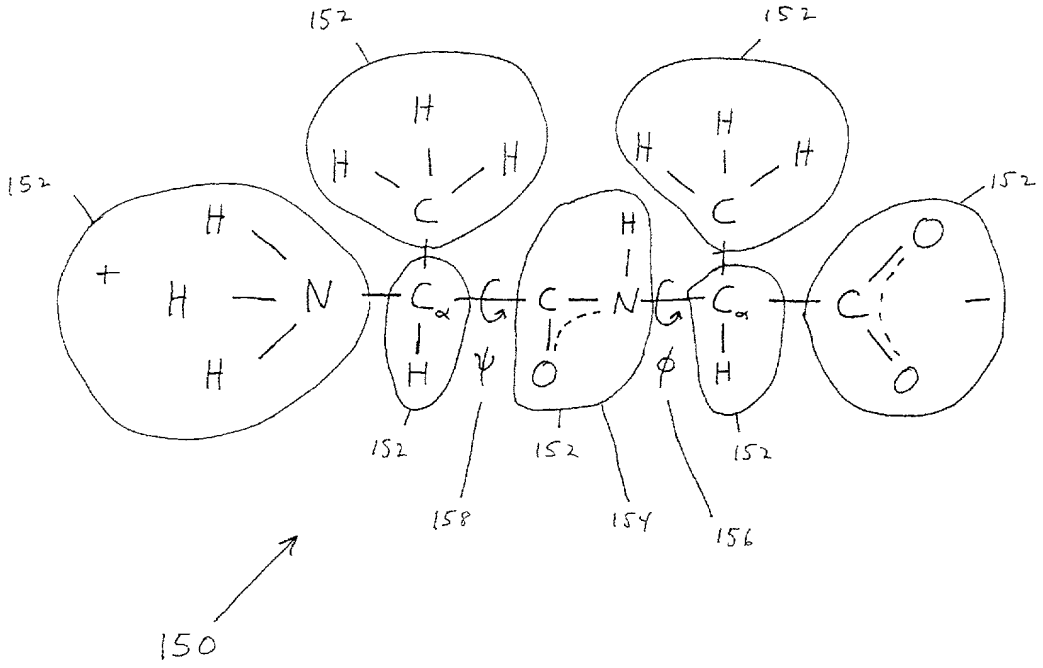

50
52
62
64
58
Modeler
Molecules
Force Field
Solvent
Biochem Components
Visualization
60
54
Physical Model
Multibody System
Analysis
Integrators
48
66
56
68

Fig. 1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156

Fig. 3

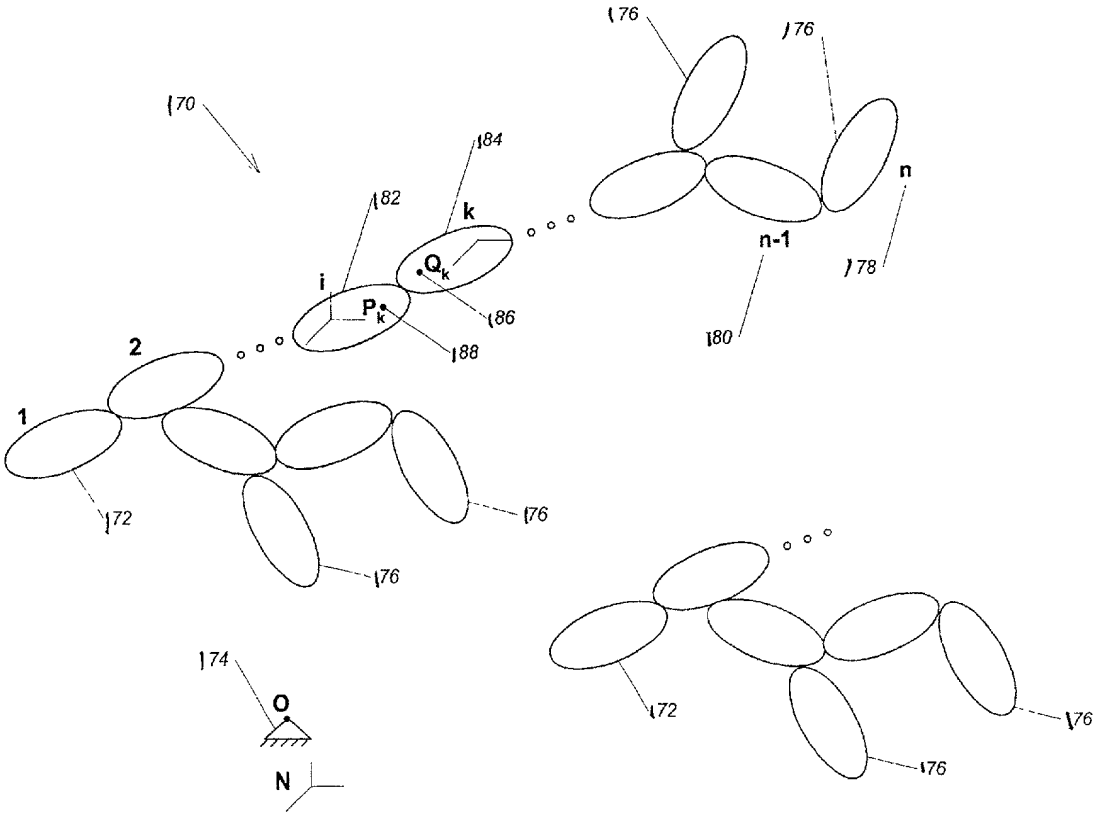
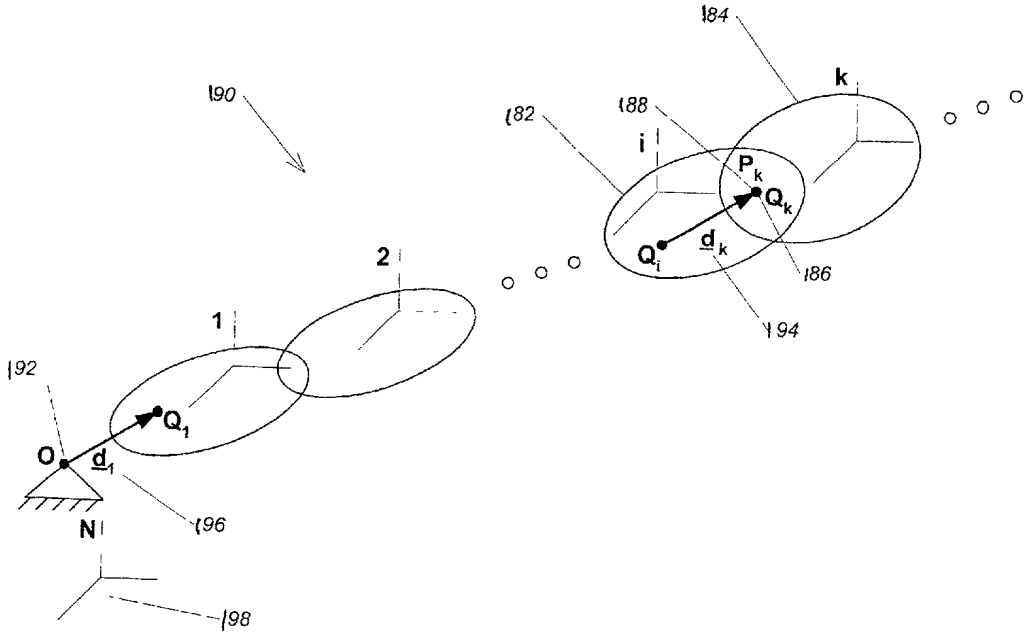

170
176
176
184
182
k
n
n-1
i
Q_k
P_k
186
188
178
180
2
1
172
176
176
174
O
N
172
176
176

Fig. 2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k
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188
i
P_k
Q_k
Q_i
d_k
186
194
2
1
192
Q_1
O
d_1
N
196
198

Fig. 3

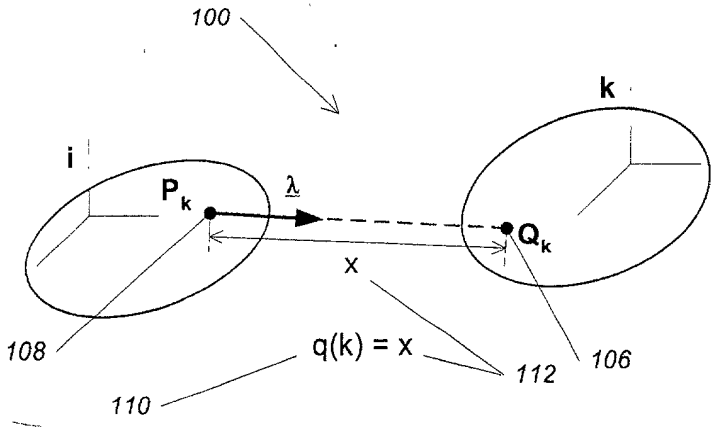


Fig. 4A

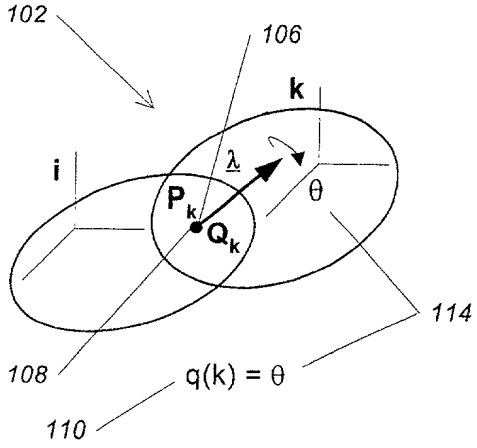


Fig. 4B

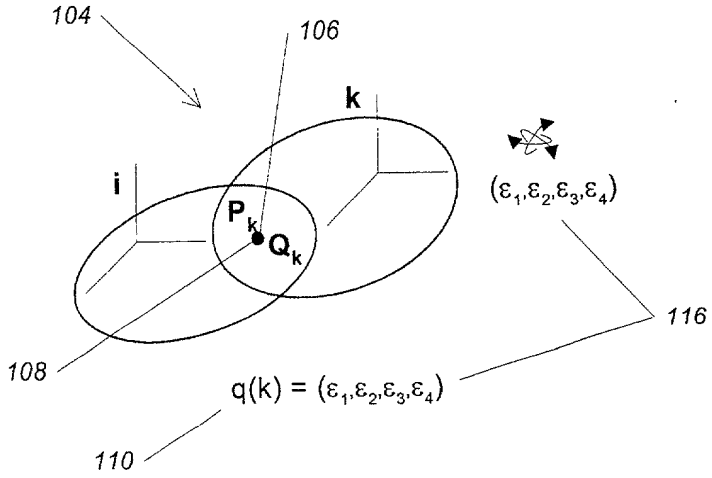
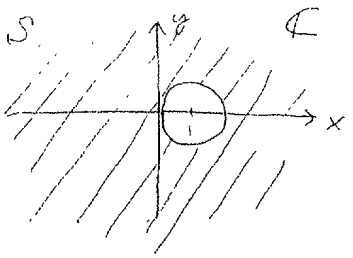


Fig. 4C

Implicit Euler

$$R(z) = \frac{1}{1-z}$$



$$\lim_{z \to \infty} R(z) = 0$$

L-Stable

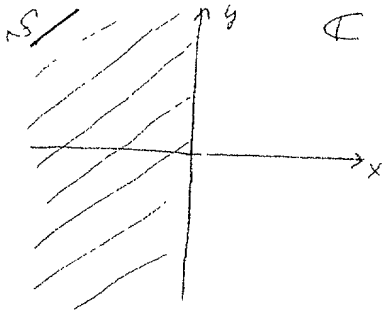
$S \supset \mathbb{C}^-$

A-Stable

Fig. 5A

Implicit Midpoint

$$R(z) = \frac{1 + z/2}{1 - z/2}$$



$$\lim_{z \to \infty} R(z) \neq 0$$

NOT L-Stable

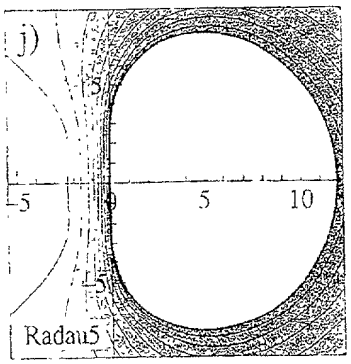
$S \supset \mathbb{C}^-$

A-Stable

Fig. 5B

Radau 5

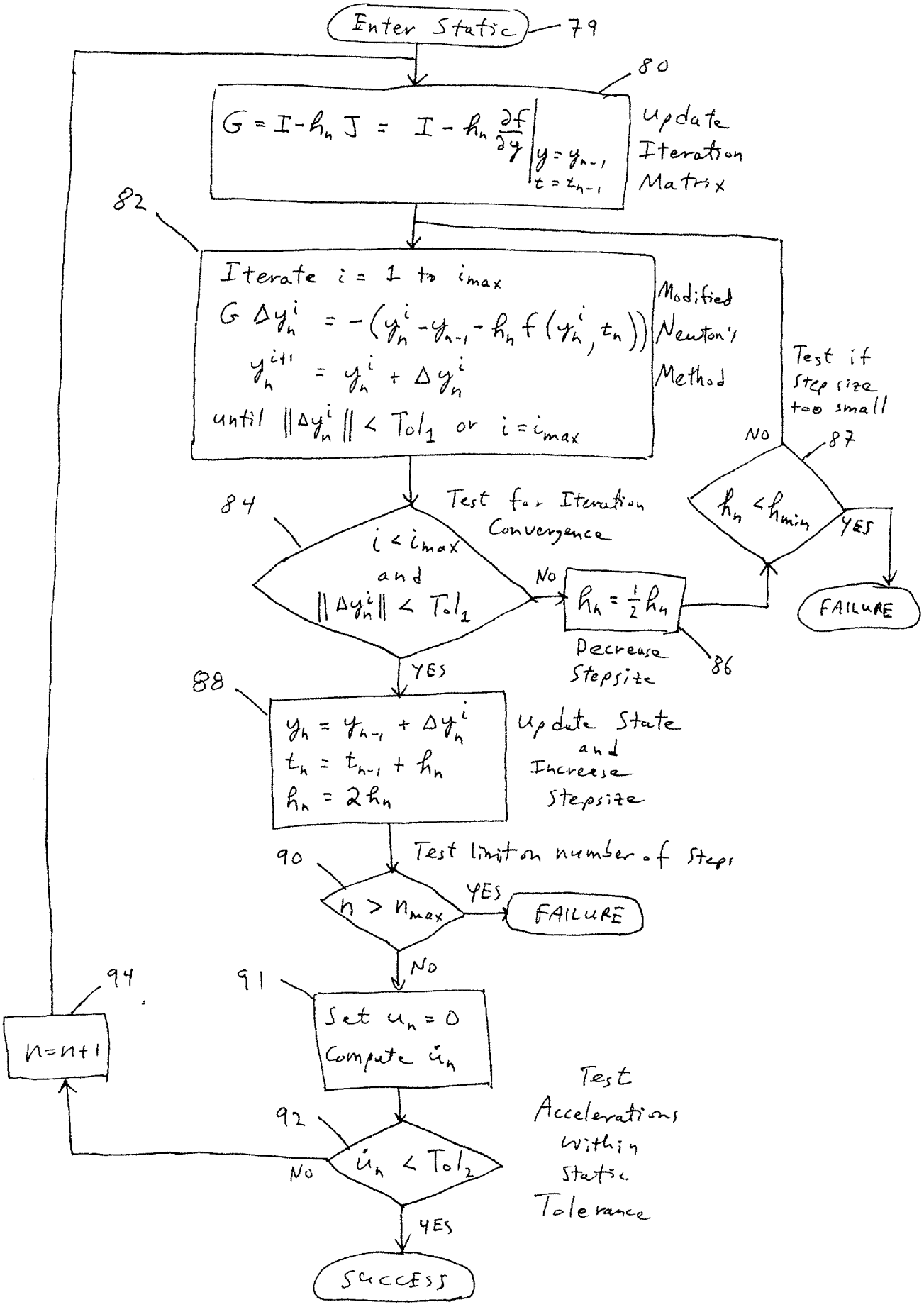
$$R(z) = \frac{1 + 2z/5 + z^2/10}{1 - 3z/5 + 3z^2/20 - z^3/60}$$



$$\lim_{z \to \infty} R(z) = 0$$

L-Stable

Fig. 5C


Enter Static
79
80
$G = I - h_n J = I - h_n \frac{\partial f}{\partial y}\Big|_{\substack{y=y_{n-1} \\ t=t_{n-1}}}$
Update Iteration Matrix
82
Iterate $i = 1$ to i_{max}
$G\,\Delta y_n^i = -(y_n^i - y_{n-1} - h_n f(y_n^i, t_n))$
$y_n^{i+1} = y_n^i + \Delta y_n^i$
until $\|\Delta y_n^i\| < Tol_1$ or $i = i_{max}$
Modified Newton's Method
Test if Step size too small
NO
87
$h_n < h_{min}$
YES
FAILURE
84
Test for Iteration Convergence
$i < i_{max}$ and $\|\Delta y_n^i\| < Tol_1$
NO
$h_n = \frac{1}{2} h_n$
Decrease Stepsize
86
YES
88
$y_n = y_{n-1} + \Delta y_n^i$
$t_n = t_{n-1} + h_n$
$h_n = 2h_n$
Update State and Increase Stepsize
90
Test limit on number of Steps
$n > n_{max}$
YES
FAILURE
NO
91
Set $u_n = 0$
Compute $\ddot{u}_n$
92
$\ddot{u}_n < Tol_2$
NO
YES
Test Accelerations within Static Tolerance
94
$n = n+1$
SUCCESS

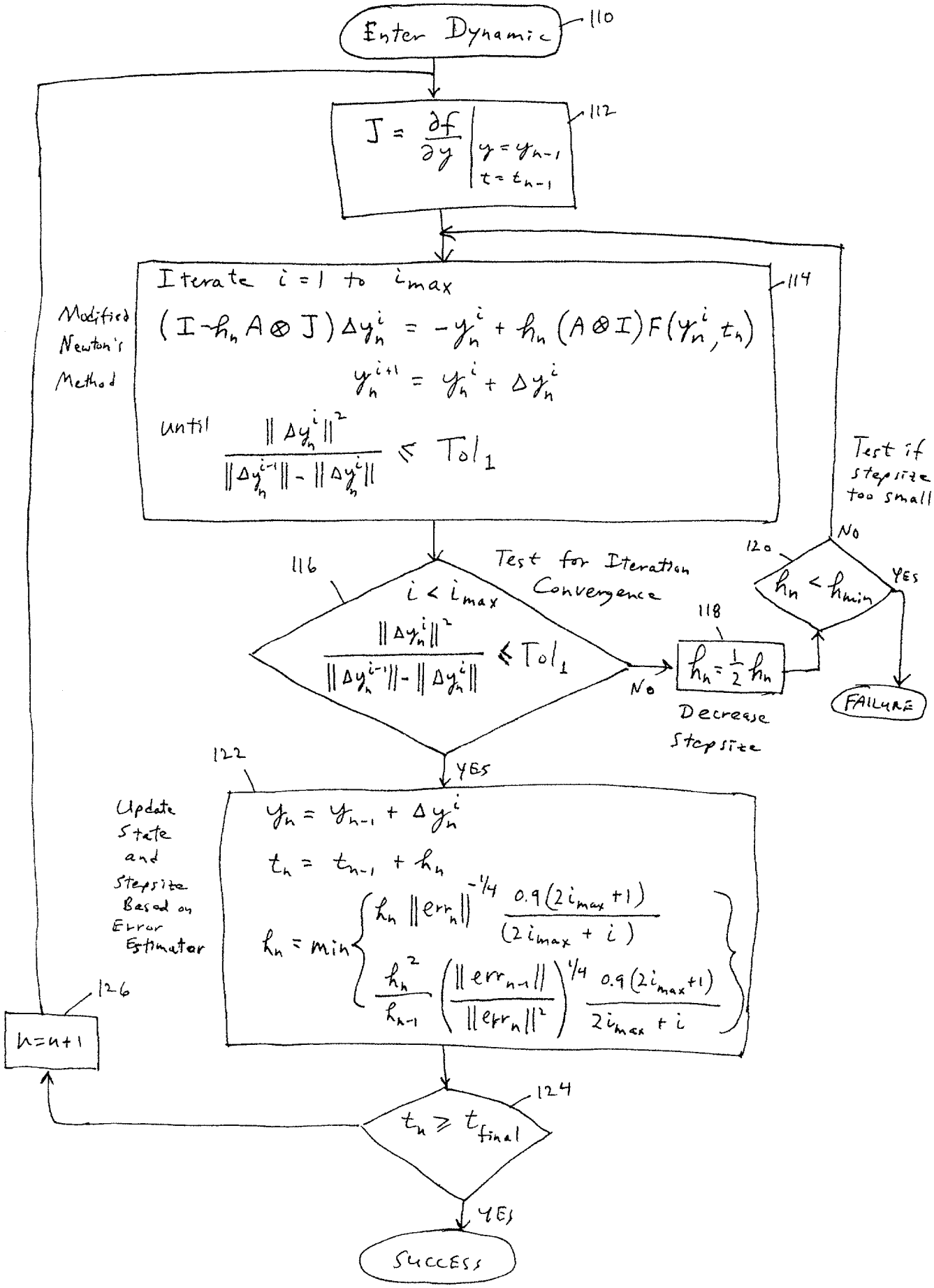
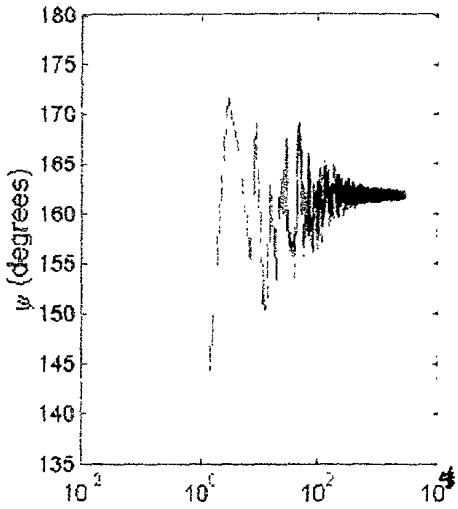
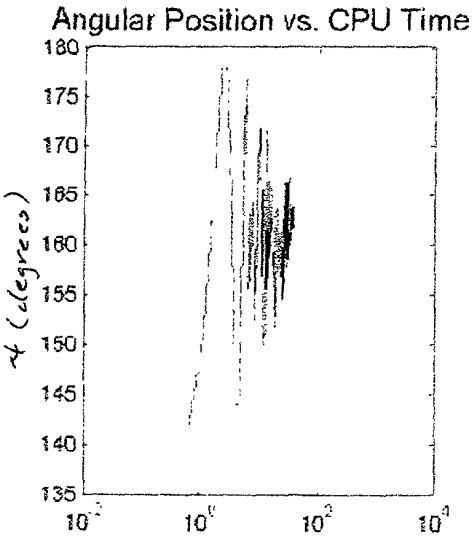

Enter Dynamic
110
$J = \frac{\partial f}{\partial y}\Big|_{\substack{y=y_{n-1} \\ t=t_{n-1}}}$
112
Iterate $i = 1$ to i_{max}
114
Modified Newton's Method
$(I - h_n A \otimes J)\Delta y_n^i = -y_n^i + h_n (A \otimes I) F(y_n^i, t_n)$
$y_n^{i+1} = y_n^i + \Delta y_n^i$
until $\frac{\|\Delta y_n^i\|^2}{\|\Delta y_n^{i-1}\| - \|\Delta y_n^i\|} \leq Tol_1$
Test if stepsize too small
120
$h_n < h_{min}$
NO
YES
FAILURE
116
Test for Iteration Convergence
$i < i_{max}$
$\frac{\|\Delta y_n^i\|^2}{\|\Delta y_n^{i-1}\| - \|\Delta y_n^i\|} \leq Tol_1$
NO
118
$h_n = \frac{1}{2} h_n$
Decrease Stepsize
YES
122
Update State and Stepsize Based on Error Estimator
$y_n = y_{n-1} + \Delta y_n^i$
$t_n = t_{n-1} + h_n$
$h_n = \min\left\{ h_n \|err_n\|^{-1/4} \frac{0.9(2i_{max}+1)}{(2i_{max}+i)}, \frac{h_n^2}{h_{n-1}} \left(\frac{\|err_{n-1}\|}{\|err_n\|^2}\right)^{1/4} \frac{0.9(2i_{max}+1)}{2i_{max}+i} \right\}$
126
$h = n+1$
124
$t_n \geq t_{final}$
YES
SUCCESS

Fig. 1



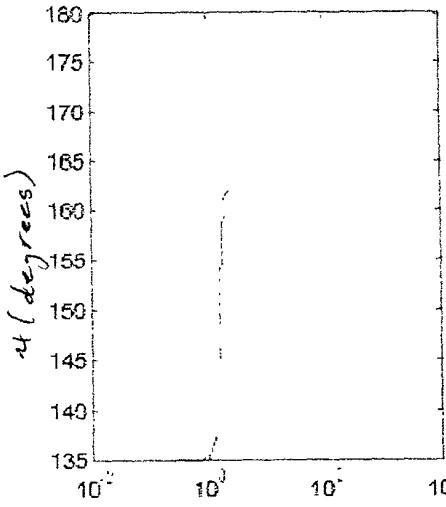
Verlet

Fig. 9A

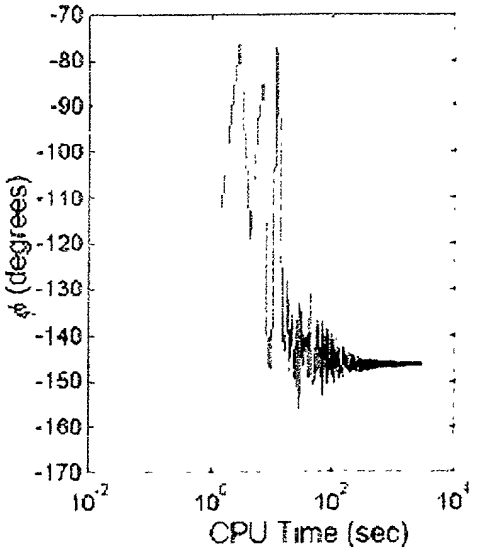


Radau5

Fig. 9B

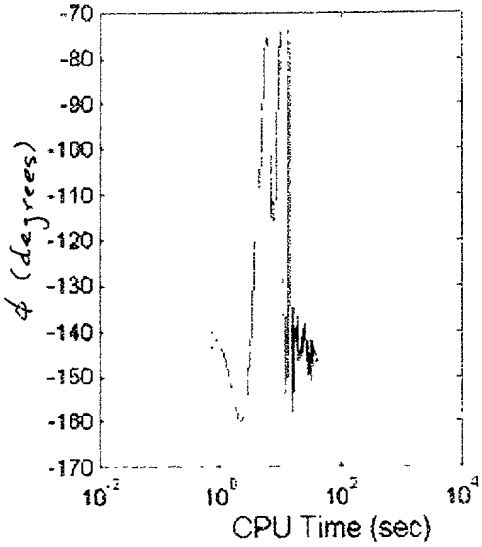


Implicit Euler



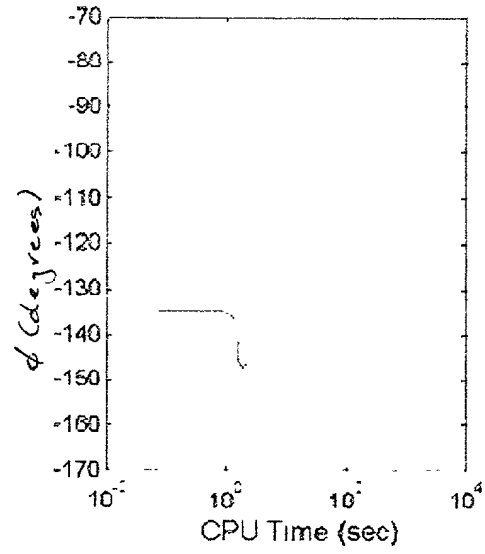
Verlet

Fig. 9D



Radau5

Fig. 9E



Implicit Euler

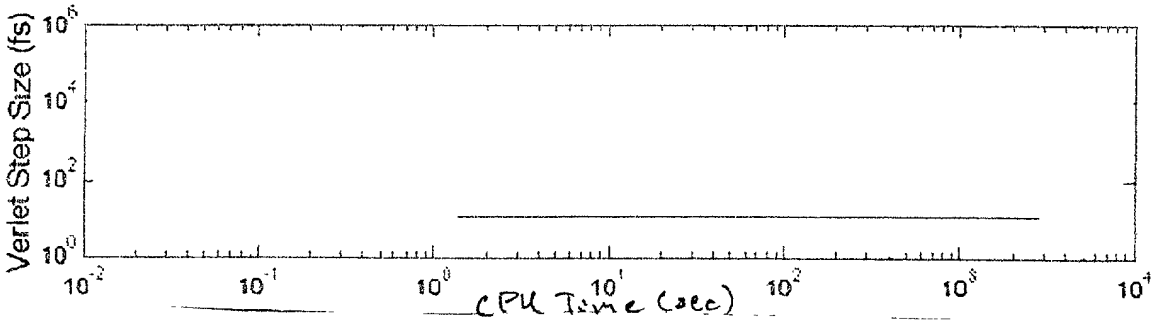


Fig. 10A

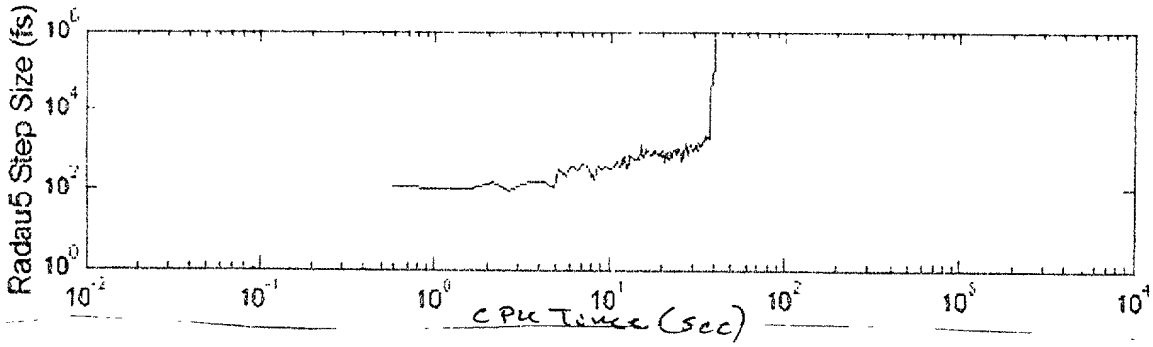


Fig. 10B

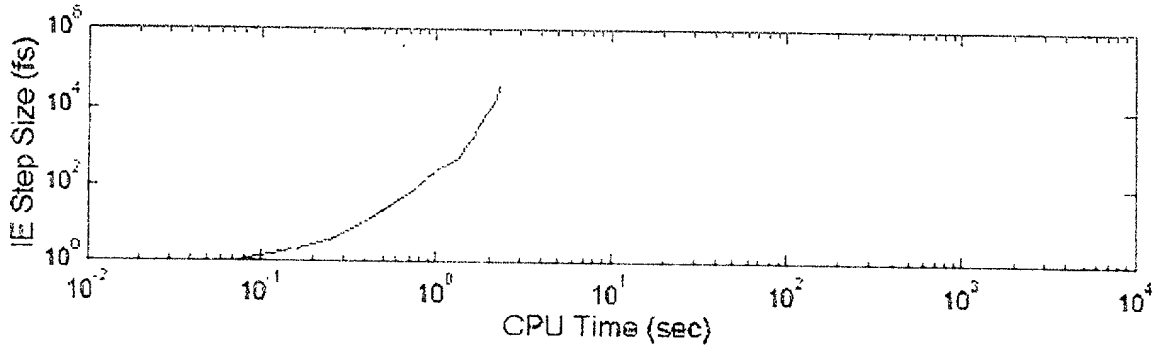


Fig. 10C